Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International! Enter x:x
LOGINID:ssspta1623paz
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Sep 29	The Philippines Inventory of Chemicals and Chemical Substances (PICCS) has been added to CHEMLIST
NEWS 3	Oct 27	New Extraction Code PAX now available in Derwent Files
NEWS 4	Oct 27	SET ABBREVIATIONS and SET PLURALS extended in Derwent World Patents Index files
NEWS 5	Oct 27	Patent Assignee Code Dictionary now available in Derwent Patent Files
NEWS 6	Oct 27	Plasdoc Key Serials Dictionary and Echoing added to Derwent Subscriber Files WPIDS and WPIX
NEWS 7	Nov 29	Derwent announces further increase in updates for DWPI
NEWS 8	Dec 5	French Multi-Disciplinary Database PASCAL Now on STN
NEWS 9	Dec 5	Trademarks on STN - New DEMAS and EUMAS Files
NEWS 10	Dec 15	2001 STN Pricing
NEWS 11	Dec 17	Merged CEABA-VTB for chemical engineering and biotechnology
NEWS 12	Dec 17	Corrosion Abstracts on STN
NEWS 13	Dec 17	SYNTHLINE from Prous Science now available on STN
NEWS 14	Dec 17	The CA Lexicon available in the CAPLUS and CA files
NEWS 15	Jan 05	AIDSLINE is being removed from STN
NEWS 16	Feb 06	Engineering Information Encompass files have new names
NEWS 17	Feb 16	TOXLINE no longer being updated

NEWS EXPRESS	FREE UPGRADE 5.0e FOR STN EXPRESS 5.0 WITH DISCOVER! (WINDOWS) NOW AVAILABLE
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 07:24:59 ON 18 APR 2001

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION

FULL ESTIMATED COST 0.15 0.15

FILE 'REGISTRY' ENTERED AT 07:25:09 ON 18 APR 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 17 APR 2001 HIGHEST RN 331714-48-8
DICTIONARY FILE UPDATES: 17 APR 2001 HIGHEST RN 331714-48-8

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

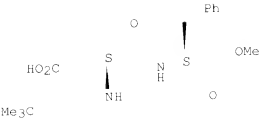
Structure search limits have been increased. See HELP SLIMIT for details.

```
=> e neotame/cn
E1            1      NEOTALL F/CN
E2            1      NEOTALL G/CN
E3            1 --> NEOTAME/CN
E4            1      NEOTAN UE 1402/CN
E5            1      NEOTAN UE 3100/CN
E6            1      NEOTARCHOCIN/CN
E7            1      NEOTEBANYL/CN
E8            1      NEOTEBEN/CN
E9            1      NEOTELOMYCIN/CN
E10           1      NEOTEMP/CN
E11           1      NEOTENINE/CN
E12           1      NEOTENONE/CN

=> s e3; d
L1            1 NEOTAME/CN


L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2001 ACS
RN   165450-17-9  REGISTRY
CN   L-Phenylalanine, N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl-, 2-methyl
ester
     (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   L-Phenylalanine, N-[N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-, 1-methyl
     ester
OTHER NAMES:
CN   Neotame
FS   STEREOSEARCH
MF   C20 H30 N2 O5
CI   COM
SR   CA
LC   STN Files:   AGRICOLA, ANABSTR, BIOSIS, CA, CAPLUS, CASREACT, CBNB, CIN,
       MRCK*, PROMT, TOXLIT, USPATFULL
         (*File contains numerically searchable property data)

Absolute stereochemistry.
```



59 REFERENCES IN FILE CA (1967 TO DATE)
9 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
59 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.92	6.07

FILE 'CAPLUS' ENTERED AT 07:26:36 ON 18 APR 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1967 - 18 Apr 2001 VOL 134 ISS 17
FILE LAST UPDATED: 17 Apr 2001 (20010417/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in CAPLUS on STN.

The CA Lexicon is now available in the Controlled Term (/CT) field. Enter HELP LEXICON for full details.

=> s l1<neotame>

SmartSELECT INITIATED
New TRANSFER and ANALYZE Commands Now Available
See HELP TRANSFER and HELP ANALYZE for Details

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COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                          ENTRY     SESSION
FULL ESTIMATED COST                                         0.33       6.40

FILE 'REGISTRY' ENTERED AT 07:26:58 ON 18 APR 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 American Chemical Society (ACS)

SET SMARTSELECT ON
SET COMMAND COMPLETED

SEL L1 1- NEOTAME
'NEOTAME' IS NOT A VALID FIELD CODE FOR FILE 'REGISTRY'
The following are valid field codes:
AF ------ Alternate Molecular Formula
AR ------ Alternate Registry Number
CCI ----- Component Substance Class Identifier
CHEM ---- CAS Registry Numbers and Selected Names
CI ------ Substance Class Identifier
CMF ----- Component Molecular Formulas
CN ------ Chemical Names (Up to 50)
CRN ----- Component Registry Numbers
DEF ----- Definition
DR ------ Deleted Registry Number
EA ------ Elemental Analysis for Ring System
ES ------ Elemental Sequence for Ring System
FCN ----- All Chemical Names
FS ------ File Segment
IN ------ CA Index Name
LC ------ CAS Registry Number Locator
MF ------ Molecular Formula
NAME ---- Selected Substance Names
PCT ----- Polymer Class Term
PR ------ Preferred Registry Number
RF ------ Ring System Formula
RID ----- Ring Identifier
RN ------ CAS Registry Number
RR ------ Replacing Registry Number
SCN ----- Short Chemical Name (IN and OTHER NAMES)
SEQ ----- Protein Sequence Display using 1 Letter Amino Acid Codes (default)
SEQ3 ---- Protein Sequence Display using 3 Letter Amino Acid Codes
SQEFP --- Protein Sequence (exact family search form)
SQEN ---- Nucleic Acid Sequence (exact search form)
SQEP ---- Protein Sequence (exact search form)
SQSFP --- Protein Sequence (subsequence family search form)
SQSN ---- Nucleic Acid Sequence (subsequence search form)
SQSP ---- Protein Sequence (subsequence search form)
SR ------ Source of Registration
SZ ------ Size for Ring System
ENTER DISPLAY CODE (CHEM) OR ?:chem
L2          SEL L1 1- CHEM :        2 TERMS

SET SMARTSELECT OFF
SET COMMAND COMPLETED

COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                          ENTRY     SESSION
```

FULL ESTIMATED COST 9.11 15.51

FILE 'CAPLUS' ENTERED AT 07:27:27 ON 18 APR 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

S L2
L3 64 L2

=> d scan l3

L3 64 ANSWERS CAPLUS COPYRIGHT 2001 ACS
IC ICM C07C229-28
ICS C07D279-04; C07D275-06; C07D315-00
NCL 560039000
CC 17-6 (Food and Feed Chemistry)
TI N-[n-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine 1-methyl ester synergistic sweetener blends
ST sweetening agent synergy dipeptide deriv; aspartame deriv sweetener synergy; **neotame** sweetener synergy
IT Sweetening agents
(N-[n-(3,3-dimethylbutyl)-l-.alpha.-aspartyl]-l-phenylalanine 1-Me ester synergistic sweetener blends)
IT Cooperative phenomena
(synergism; N-[n-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine 1-Me ester synergistic sweetener blends)
IT 57-50-1, Sucrose, biological studies 81-07-2, Saccharin 22839-47-0, Aspartame 55589-62-3, Acesulfamepotassium **165450-17-9, Neotame**
RL: BAC (Biological activity or effector, except adverse); FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(N-[n-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine 1-Me ester synergistic sweetener blends)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L3 64 ANSWERS CAPLUS COPYRIGHT 2001 ACS
IC ICM C07C229-00
NCL 560040000
CC 34-3 (Amino Acids, Peptides, and Proteins)
TI Method for preparing and purifying an N-alkylated aspartame derivative
ST aspartame dimethylbutyl prepn purifn
IT **165450-17-9P**
RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and purifn. of N-alkylated aspartame deriv.)
IT 2987-16-8, 3,3-Dimethylbutyraldehyde 22839-47-0, Aspartame
RL: RCT (Reactant)
(prepn. and purifn. of N-alkylated aspartame deriv.)

L3 64 ANSWERS CAPLUS COPYRIGHT 2001 ACS
CC 17-0 (Food and Feed Chemistry)
TI **Neotame**: discovery, properties, utility
ST review **neotame** sweetener property use
IT Sweetening agents
(noncariogenic, noncaloric, nonnutritive; **Neotame** discovery, properties, and utility as)
IT **165450-17-9, Neotame**
RL: BAC (Biological activity or effector, except adverse); FFD (Food or feed use); PRP (Properties); BIOL (Biological study); USES (Uses)

(discovery, properties, and utility as sweetener)

L3 64 ANSWERS CAPLUS COPYRIGHT 2001 ACS
IC ICM A23L001-236
ICS A23L001-22; C07K005-075
CC 17-6 (Food and Feed Chemistry)
TI Sweetener for improving taste
ST aspartame acesulfame amino acid deriv sweetener
IT Sweetening agents
(contg. aspartame and acesulfame K and amino acid deriv.)
IT Beverages
(contg. aspartame and acesulfame K and amino acid deriv. as sweetener)
IT **165450-17-9**
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(sweetener contg. aspartame and acesulfame K and)
IT 22839-47-0, Aspartame 33665-90-6, Acesulfame
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(sweetener contg. aspartame and acesulfame K and amino acid deriv.)

L3 64 ANSWERS CAPLUS COPYRIGHT 2001 ACS
IC ICM C07K005-075
CC 17-1 (Food and Feed Chemistry)
TI Crystallization processes of stable crystals of aspartame derivatives
ST crystn aspartame deriv sweetener
IT **165450-17-9 165450-17-9D**, derivs.
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(crystn. of stable aspartame)
IT 67-56-1, Methanol, uses
RL: NUU (Nonbiological use, unclassified); USES (Uses)
(in crystn. of stable aspartame)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d his

(FILE 'HOME' ENTERED AT 07:24:59 ON 18 APR 2001)

FILE 'REGISTRY' ENTERED AT 07:25:09 ON 18 APR 2001
E NEOTAME/CN
L1 1 S E3

FILE 'CAPLUS' ENTERED AT 07:26:36 ON 18 APR 2001

FILE 'REGISTRY' ENTERED AT 07:26:58 ON 18 APR 2001
SET SMARTSELECT ON
L2 SEL L1 1- CHEM : 2 TERMS
SET SMARTSELECT OFF

FILE 'CAPLUS' ENTERED AT 07:27:27 ON 18 APR 2001
L3 64 S L2

=> s anhydrous(1)L3
6392 ANHYDROUS
L4 0 ANHYDROUS(L)L3

=> s dry (1) L3
234680 DRY
930 DRIES
23 DRYS
235429 DRY
(DRY OR DRIES OR DRYS)

```
L5            3 DRY (L) L3

=> d l5 1-3 ti

L5   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2001 ACS
TI   Neotame: discovery, properties, utility

L5   ANSWER 2 OF 3  CAPLUS  COPYRIGHT 2001 ACS
TI   The use of cyclodextrin to stabilize N-[N-(3,3-dimethylbutyl)-L-.alpha.-
     aspartyl]-L-phenylalanine 1-methyl ester

L5   ANSWER 3 OF 3  CAPLUS  COPYRIGHT 2001 ACS
TI   Neotame sweetener for dairy products and dairy product substitutes


=> d l5 1-3 ti fbib abs

L5   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2001 ACS
TI   Neotame: discovery, properties, utility
AN   2000:256584  CAPLUS
DN   133:16459
TI   Neotame: discovery, properties, utility
AU   Nofre, Claude; Tinti, Jean-Marie
CS   Lyon, F-69008, Fr.
SO   Food Chem. (2000), 69(3), 245-257
     CODEN: FOCHDJ; ISSN: 0308-8146
PB   Elsevier Science Ltd.
DT   Journal; General Review
LA   English
AB   A review with 39 refs.  Neotame (NTM) is a new nonnutritive
     sweetener.  NTM is a deriv. of aspartame (APM).  NTM has a clean sweet
     taste and a good flavor profile.  It is a high-potency sweetener: it is
     6000-10,000 times sweeter than sucrose and 30-60 times sweeter than APM.
     NTM is a noncaloric, noncariogenic sweetener.  NTM has an extensive shelf
     life in dry conditions.  In aq. food systems, it presents the
     same functionalities as APM in acidic medium, but it is significantly
more
     stable in neutral medium.  Consequently, NTM should be a useful sweetener
     in baked goods.  NTM is compatible with reducing sugars and
aldehyde-based
     flavoring agents.  It has flavor-enhancing properties.  Its relative cost
     is expected to be lower than sucrose or APM at sweetness equivalence.  A
     petition was filed in the USA in Dec. 1998 for its approval as a
     general-use sweetener; other regulatory activities are underway in
several
     countries.
RE.CNT  39
RE
(3) Beck, C; Low calorie and special dietary foods 1978, P59 CAPLUS
(7) Homler, B; Aspartame: physiology and biochemistry 1984, P247 CAPLUS
(8) Ketelsen, S; Journal of Food Science 1993, V58, P1418 CAPLUS
(10) Lindinger, W; Alcoholism Clinical and Experimental Research 1997, V21,
    P939 CAPLUS
(13) Mazur, R; Developments in sweeteners 1979, P125 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5   ANSWER 2 OF 3  CAPLUS  COPYRIGHT 2001 ACS
TI   The use of cyclodextrin to stabilize N-[N-(3,3-dimethylbutyl)-L-.alpha.-
     aspartyl]-L-phenylalanine 1-methyl ester
AN   2000:190872  CAPLUS
DN   132:221731
```

TI The use of cyclodextrin to stabilize N-[N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine 1-methyl ester
IN Bishay, Ihab E.; Fotos, Jim G.; Desai, Nitin; Cleary, Michael; Schroeder, Steve
PA The Nutrasweet Company, USA
SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000015049	A1	20000323	WO 1999-US21471	19990916
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			US 1998-100867	19980917
AU 9961504	A1	20000403	AU 1999-61504	19990916
			US 1998-100867	19980917
			WO 1999-US21471	19990916

AB N-[N-(3,3-Dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine 1-Me ester (**neotame** sweetener) is combined with cyclodextrin to form compns. exhibiting increased stability and soly. The cyclodextrin may be .alpha., .beta. or .gamma., or a mixt. of these, and may be substituted or unsubstituted. This stabilized complex can be used in a variety of applications. Thus, a carbonated cola contains 1.632 g cyclodextrin-**neotame** complex (5:1) in 977 g water, plus other ingredients. Complex formation can be accomplished by a variety of methods, such as co-pptn., slurry complexation, paste complexation, mixing and heating, extrusion, **dry** mixing, wet pelletization, agglomeration and other methods.

RE.CNT 3
RE
(1) Majid; US 5070081 A 1991 CAPLUS
(2) Nofre; US 5480668 A 1996 CAPLUS
(3) Ojima; EP 0097950 A 1984 CAPLUS

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2001 ACS
TI Neotame sweetener for dairy products and dairy product substitutes
AN 1999:404813 CAPLUS
DN 131:31305
TI Neotame sweetener for dairy products and dairy product substitutes
IN Gaughan, Wanda M.; Gerlat, Paula A.; Ziegler, Jeanette G.; Walters, Gale C.; Logli, Lori; Corliss, Glenn; Finley, John
PA The Nutrasweet Company, USA
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9930578	A1	19990624	WO 1998-US27176	19981217
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,				

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            DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG,
            KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,
            NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
            UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
            CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                            US 1997-69952     19971217
    AU 9919364        A1   19990705         AU 1999-19364     19981217
                                            US 1997-69952     19971217
                                            WO 1998-US27176   19981217

AB  N-[N-(3,3-Dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine 1-Me ester (
    neotame) is used to sweeten dairy products, including milk (from
    various species and of various milk fat content), enzyme treated milk,
    filled milk, cream, creamers, cultured milk, milk concs., dry
    milk, fluid and dried whey, fluid and dry milk based desserts
    and beverages, and fluid and dry aerated desserts and toppings.
    The dairy products also include frozen cultured milk products, such as
    frozen yogurt, and frozen fluid dairy products, such as ice cream, ice
    milk, sherbet, custards and french ice cream, mellorine, novelties, and
    the like.  Dairy analog products include soy milk, soy powder,
caseinates,
    and non-dairy coffee whiteners, as well as frozen products such as sorbet
    and non-dairy novelties.  Thus, an orange sherbet may be sweetened with
20
    ppm neotame.
RE.CNT  6
RE
(1) Ajinomoto; WO 9839979 A 1998 CAPLUS
(2) Ajinomoto; WO 9839979 A 1998 CAPLUS
(3) Nofre, C; WO 9530689 A 1995 CAPLUS
(4) Nofre, C; US 5480668 A 1996 CAPLUS
(5) Oshawa Group; CA 1267030 A 1990
ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> logoff hold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     15.18      30.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     -1.76      -1.76

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:30:30 ON 18 APR 2001

Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International!  Enter x:x
LOGINID:ssspta1623paz
PASSWORD:
  * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 07:53:26 ON 18 APR 2001
FILE 'CAPLUS' ENTERED AT 07:53:26 ON 18 APR 2001
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
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                                                          ENTRY     SESSION
FULL ESTIMATED COST                                       15.18       30.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                          ENTRY     SESSION
CA SUBSCRIBER PRICE                                       -1.76      -1.76

=> d his

     (FILE 'HOME' ENTERED AT 07:24:59 ON 18 APR 2001)

     FILE 'REGISTRY' ENTERED AT 07:25:09 ON 18 APR 2001
               E NEOTAME/CN
L1             1 S E3

     FILE 'CAPLUS' ENTERED AT 07:26:36 ON 18 APR 2001

     FILE 'REGISTRY' ENTERED AT 07:26:58 ON 18 APR 2001
               SET SMARTSELECT ON
L2           SEL L1 1- CHEM :       2 TERMS
               SET SMARTSELECT OFF

     FILE 'CAPLUS' ENTERED AT 07:27:27 ON 18 APR 2001
L3            64 S L2
L4             0 S ANHYDROUS(L)L3
L5             3 S DRY (L) L3

=> s l3 and stability
         436415 STABILITY
          17851 STABILITIES
         445166 STABILITY
                (STABILITY OR STABILITIES)
L6             7 L3 AND STABILITY

=> d l6 1-7 ti

L6   ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   Structure, Dynamics, and Stability of .beta.-Cyclodextrin
     Inclusion Complexes of Aspartame and Neotame

L6   ANSWER 2 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   Cereals and cereal-based food sweetened with neotame

L6   ANSWER 3 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   Method for preparing crystal of aspartame derivative excellent in
     stability

L6   ANSWER 4 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   Discovery and development of neotame

L6   ANSWER 5 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   The use of cyclodextrin to stabilize N-[N-(3,3-dimethylbutyl)-L-.alpha.-
     aspartyl]-L-phenylalanine 1-methyl ester

L6   ANSWER 6 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   Low-calorie granular sweeteners containing dextrin with high dietary
fiber
     content

L6   ANSWER 7 OF 7  CAPLUS  COPYRIGHT 2001 ACS
TI   New dipeptide derivatives and analogs useful as sweetening agents, and
```

process for their preparation

=> d l6 3,4,7 ti fbib abs

L6 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2001 ACS
TI Method for preparing crystal of aspartame derivative excellent in **stability**
AN 2000:314716 CAPLUS
DN 132:321238
TI Method for preparing crystal of aspartame derivative excellent in **stability**
IN Kawahara, Shigeru; Kishishita, Akihiro; Nagashima, Kazutaka; Takemoto, Tadashi
PA Ajinomoto Co., Inc., Japan
SO PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000026235	A1	20000511	WO 1999-JP6083	19991101
W: BR, CA, CN, HU, JP, KR, MX, RU, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
			JP 1998-310227	19981030
			JP 1998-310228	19981030
JP 2000136198	A2	20000516	JP 1998-310228	19981030

AB A method for prepg. the A type crystal of N-(3,3-dimethylbutyl)-APM being excellent in **stability**, comprises holding the B type crystal thereof under a controlled condition with an abs. humidity of 0.203 kg/kg or lower and a material temp. of 25.degree. to 80.degree., to thereby produce crystal transition, including a method for prepg. the A type crystal of N-(3,3-dimethylbutyl)-APM. holding the D type crystal thereof under a controlled condition with an abs. humidity of 0.0550 kg/kg or lower and a material temp. of 25.degree. to 80.degree., to thereby causing crystal transition. These crystal transition methods allow the prepn. of a crystal excellent in **stability** in a cost-effective manner.
RE.CNT 15
RE
(1) Ajinomoto Co Inc; JP 02243699 A CAPLUS
(2) Ajinomoto Co Inc; US 5543544 A CAPLUS
(4) Ajinomoto Co Inc; EP 362706 A1 1990 CAPLUS
(7) Nofre Claude; FR 2719590 A CAPLUS
(8) Nofre Claude; FR 2719591 A CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2001 ACS
TI Discovery and development of **neotame**
AN 2000:250511 CAPLUS
DN 132:292833
TI Discovery and development of **neotame**
AU Witt, John
CS Nutrition and Consumer Sector, Monsanto Company, Mt. Prospect, IL, USA
SO World Rev. Nutr. Diet. (1999), 85(Low-Calorie Sweeteners), 52-57
CODEN: WRNDAT; ISSN: 0084-2230
PB S. Karger AG
DT Journal; General Review
LA English

AB A review without refs., describing development and characterization of **neotame**, sweetness potency and flavor profile of **neotame** in water, and application, functionality, and sweetness level and **stability** of **neotame**.

L6 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2001 ACS
TI New dipeptide derivatives and analogs useful as sweetening agents, and process for their preparation
AN 1995:701729 CAPLUS
DN 123:84006
TI New dipeptide derivatives and analogs useful as sweetening agents, and process for their preparation
IN Nofre, Claude; Tinti, Jean Marie
PA Fr.
SO Fr. Demande, 23 pp.
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2697844	A1	19940513	FR 1992-13615	19921112
	FR 2697844	B1	19950127		
	US 5480668	A	19960102	US 1993-149365	19931109
				FR 1992-13615	19921112
	CA 2139233	AA	19940526	CA 1993-2139233	19931110
				FR 1992-13615	19921112
	WO 9411391	A1	19940526	WO 1993-FR1103	19931110
	W: AU, BB, BG, BR, BY, CA, CZ, FI, HU, JP, KP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
				FR 1992-13615	19921112
	AU 9454681	A1	19940608	AU 1994-54681	19931110
	AU 664663	B2	19951123		
				FR 1992-13615	19921112
				WO 1993-FR1103	19931110
	LT 3142	B	19950131	LT 1993-1457	19931110
				FR 1992-13615	19921112
	EP 669935	A1	19950906	EP 1994-900182	19931110
	EP 669935	B1	19960605		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
				FR 1992-13615	19921112
				WO 1993-FR1103	19931110
	HU 72192	A2	19960328	HU 1994-3842	19931110
	HU 218158	B	20000628		
				FR 1992-13615	19921112
	JP 08503206	T2	19960409	JP 1993-511787	19931110
				FR 1992-13615	19921112
				WO 1993-FR1103	19931110
	AT 138935	E	19960615	AT 1994-900182	19931110
				FR 1992-13615	19921112
	ES 2091114	T3	19961016	ES 1994-900182	19931110
				FR 1992-13615	19921112
	RO 112621	B1	19971128	RO 1994-2023	19931110
				FR 1992-13615	19921112
				WO 1993-FR1103	19931110
	RU 2107071	C1	19980320	RU 1994-46457	19931110
				FR 1992-13615	19921112
				WO 1993-FR1103	19931110

IL 107551	A1	19980816	IL 1993-107551	19931110
			FR 1992-13615	19921112
CZ 285018	B6	19990512	CZ 1994-3319	19931110
			FR 1992-13615	19921112
SK 280180	B6	19990910	SK 1994-1586	19931110
			FR 1992-13615	19921112
			WO 1993-FR1103	19931110
PL 177090	B1	19990930	PL 1993-306841	19931110
			FR 1992-13615	19921112
			WO 1993-FR1103	19931110
ZA 9308430	A	19940613	ZA 1993-8430	19931111
			FR 1992-13615	19921112
CN 1090571	A	19940810	CN 1993-114462	19931112
CN 1038747	B	19980617		
			FR 1992-13615	19921112
FI 9405451	A	19941222	FI 1994-5451	19941121
			FR 1992-13615	19921112
			WO 1993-FR1103	19931110
NO 9405090	A	19941230	NO 1994-5090	19941230
			FR 1992-13615	19921112
			WO 1993-FR1103	19931110

OS CASREACT 123:84006; MARPAT 123:84006
GI For diagram(s), see printed CA Issue.
AB Title compds. I [R = C4-13 (un)satd. (a)cyclic hydrocarbyl; n = 1 or 2; Y = CO2Me, CO2Et, Me, CH2OH, CONMe2, Ph, 2-furyl, H; Z = CH2Ph, Ph, Bu, CO2Me, CO2Et, CO2Pr, fenchyloxycarbonyl, CONHR'; R' = Me, Et, Pr, isoamyl, CHMeCO2Me, dicyclopropylmethyl, 2,2,4,4-tetramethyl-3-thietanyl, etc.] are claimed, and are useful as sweeteners. I include aspartame (II) derivs., and show both higher sweetening power and increased **stability** vs. II. For example, reductive alkylation of aspartame by com. Me3CCH2CHO and NaBH3CN in MeOH at room temp. gave 62% title compd. III. Tested as aq. solns., the sweetening power of III was approx. 80-fold that of II. Also, in aq. soln. at pH 3 and 70.degree., the half-life of III was 55 h, vs. 24 h for II. Sweetening and/or **stability** data for some of the other claimed I are also reported.

=>

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	27.77	43.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.53	-3.53

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LAST RELOADED: Apr 13, 2001 (20010413/UP).

=>

NAME	CREATED	NOTES/TITLE
AMINOPOLY/A	16 APR 2001	231 ANSWERS IN FILE CAPLUS

TWOAMINOPOLY/Q 16 APR 2001 UPLOADED STRUCTURE

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NO SAVED SDI REQUESTS

=>

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.00	43.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.53

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FILE COVERS 1967 - 18 Apr 2001 VOL 134 ISS 17
FILE LAST UPDATED: 17 Apr 2001 (20010417/ED)

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.33	43.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.53

FILE 'STNGUIDE' ENTERED AT 07:58:56 ON 18 APR 2001

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Apr 13, 2001 (20010413/UP).

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.00	43.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.53

FILE 'CAPLUS' ENTERED AT 07:59:41 ON 18 APR 2001
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FILE LAST UPDATED: 17 Apr 2001 (20010417/ED)

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=>
ANSWER SET L3 HAS BEEN SAVED AS 'NEOTAME/A'

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.33	43.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION

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CA SUBSCRIBER PRICE                                          0.00       -3.53

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:00:12 ON 18 APR 2001

Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International!  Enter x:x
LOGINID:ssspta1623paz
PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 08:02:19 ON 18 APR 2001
FILE 'CAPLUS' ENTERED AT 08:02:19 ON 18 APR 2001
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COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                        0.33      43.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                        0.00      -3.53

=> d his

     (FILE 'HOME' ENTERED AT 07:24:59 ON 18 APR 2001)

     FILE 'REGISTRY' ENTERED AT 07:25:09 ON 18 APR 2001
                E NEOTAME/CN
L1             1 S E3

     FILE 'CAPLUS' ENTERED AT 07:26:36 ON 18 APR 2001

     FILE 'REGISTRY' ENTERED AT 07:26:58 ON 18 APR 2001
                SET SMARTSELECT ON
L2           SEL L1 1- CHEM :       2 TERMS
                SET SMARTSELECT OFF

     FILE 'CAPLUS' ENTERED AT 07:27:27 ON 18 APR 2001
L3            64 S L2
L4             0 S ANHYDROUS(L)L3
L5             3 S DRY (L) L3
L6             7 S L3 AND STABILITY

     FILE 'STNGUIDE' ENTERED AT 07:58:29 ON 18 APR 2001

     FILE 'CAPLUS' ENTERED AT 07:58:49 ON 18 APR 2001

     FILE 'STNGUIDE' ENTERED AT 07:58:56 ON 18 APR 2001

     FILE 'CAPLUS' ENTERED AT 07:59:41 ON 18 APR 2001
                SAVE L3 NEOTAME/A

=> s L3 and polycrystal?
         29723 POLYCRYSTAL?
L7           0 L3 AND POLYCRYSTAL?

=> s amorphous (1) l3
        175190 AMORPHOUS
```

```
L8              2 AMORPHOUS (L) L3

=> d l8 1-2 ti fbib abs

L8   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2001 ACS
TI   Amorphous N-[N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine
     1-methyl ester
AN   2000:368409  CAPLUS
DN   133:4399
TI   Amorphous N-[N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-phenylalanine
     1-methyl ester
IN   Schroeder, Steve A.; Wang, Run
PA   The Nutrasweet Company, USA
SO   PCT Int. Appl., 24 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.         KIND  DATE           APPLICATION NO.  DATE
     ---------------    ----  --------       ---------------  --------
PI   WO 2000031118      A1    20000602       WO 1999-US27363  19991119
         W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                            US 1998-109391   19981120
AB   Amorphous N-[N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl]-L-
     phenylalanine 1-Me ester (the sweetener neotame) was prepd. by a
     process comprising melting and then cooling the melt.  Thus,
     neotame was heated slowly past its m.p. of about 82.degree. until
     a temp. of about 92.degree. was reached.  The neotame was then
     cooled to room temp. and ground to a cryst. powder.  Amorphous
     neotame has improved soly. and dissoln. properties compared to the
     known monohydrate.
RE.CNT  3
RE
(1) Leung, S; JOURNAL OF PHARMACEUTICAL SCIENCES 1998, V87(4), P508 CAPLUS
(2) Padden, B; ANALYTICAL CHEMISTRY 1999, V71(16), P3325 CAPLUS
(3) Prakash; US 5728862 A 1998 CAPLUS

L8   ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2001 ACS
TI   Crystal structure and physical characterization of neotame methanol
     solvate
AN   2000:258873  CAPLUS
DN   133:59068
TI   Crystal structure and physical characterization of neotame methanol
     solvate
AU   Dong, Zedong; Young, Victor G., Jr.; Padden, Brian E.; Schroeder, Steve
     A.; Prakash, Indra; Munson, Eric J.; Grant, David J. W.
CS   Department of Pharmaceutics, College of Pharmacy, University of
Minnesota,
     Minneapolis, MN, 55455-0343, USA
SO   J. Chem. Crystallogr. (1999), 29(8), 967-975
     CODEN: JCCYEV; ISSN: 1074-1542
PB   Kluwer Academic/Plenum Publishers
DT   Journal
```

LA English
AB The crystal structure of the methanol solvate (empirical formula: 2C20H30N2O5.cntdot.3MeOH) of the dipeptide sweetener **neotame**, N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl-L-phenylalanine Me ester, was detd. [a = 9.8989(1), b = 18.1331(1), c = 27.5725(1) .ANG., orthorhombic, space group P212121, Z = 4]. Each unit cell includes 8 **neotame** and 12 MeOH mols. Disorder exists in one **neotame** mol. and one MeOH mol. The crystals were characterized by the following techniques: hot-stage microscopy (HSM), Karl-Fischer titrimetry (KFT), powder x-ray diffractometry (PXRD), differential scanning calorimetry (DSC), thermogravimetry (TGA), and 13C solid-state NMR (SSNMR). Under HSM at a heating rate of 10.degree./min, the sample melts at 64-84.degree. and liberates bubbles at 71-86.degree.. DSC in open pans shows two overlapping endotherms at 56 and 71.degree., probably due to melting and desolvation, resp. TGA in open pans shows 5.9% wt. loss due to desolvation below 70.degree.. Under 23 mmHg over P4O10 at 23.degree., the
MeOH solvate produces pure **amorphous** anhydrate, which converts to cryst. **neotame**.H2O in the presence of moisture.
RE.CNT 21
RE
(1) Andrew, E; Prog NMR Spec 1971, V8, P1 CAPLUS
(3) Anon; US 5728862 CAPLUS
(5) Blessing, R; Acta Crystallogr 1995, VA51, P33 CAPLUS
(6) Dixon, W; J Magn Res 1982, V49, P341 CAPLUS
(7) Goodman, M; J Peptide Sci 1998, V4, P229 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.06	53.67

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.18	-4.71

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Welcome to STN International! Enter x:x
LOGINID:sssptal623paz
PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 08:47:24 ON 18 APR 2001
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.06	53.67

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.18	-4.71

```
=> d his

     (FILE 'HOME' ENTERED AT 07:24:59 ON 18 APR 2001)

     FILE 'REGISTRY' ENTERED AT 07:25:09 ON 18 APR 2001
                E NEOTAME/CN
L1             1 S E3

     FILE 'CAPLUS' ENTERED AT 07:26:36 ON 18 APR 2001

     FILE 'REGISTRY' ENTERED AT 07:26:58 ON 18 APR 2001
                SET SMARTSELECT ON
L2           SEL L1 1- CHEM :       2 TERMS
                SET SMARTSELECT OFF

     FILE 'CAPLUS' ENTERED AT 07:27:27 ON 18 APR 2001
L3            64 S L2
L4             0 S ANHYDROUS(L)L3
L5             3 S DRY (L) L3
L6             7 S L3 AND STABILITY

     FILE 'STNGUIDE' ENTERED AT 07:58:29 ON 18 APR 2001

     FILE 'CAPLUS' ENTERED AT 07:58:49 ON 18 APR 2001

     FILE 'STNGUIDE' ENTERED AT 07:58:56 ON 18 APR 2001

     FILE 'CAPLUS' ENTERED AT 07:59:41 ON 18 APR 2001
                SAVE L3 NEOTAME/A
L7             0 S L3 AND POLYCRYSTAL?
L8             2 S AMORPHOUS (L) L3

=> s l3 and anhydrate
            326 ANHYDRATE
             35 ANHYDRATES
            353 ANHYDRATE
                (ANHYDRATE OR ANHYDRATES)
L9            2 L3 AND ANHYDRATE

=> d l9 1-2 ti fbib abs

L9   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2001 ACS
TI   Investigation of Polymorphism in Aspartame and Neotame Using
     Solid-State NMR Spectroscopy
AN   2000:620337  CAPLUS
DN   133:349355
TI   Investigation of Polymorphism in Aspartame and Neotame Using
     Solid-State NMR Spectroscopy
AU   Zell, M. T.; Padden, B. E.; Grant, D. J. W.; Schroeder, S. A.;
Wachholder,
     K. L.; Prakash, I.; Munson, E. J.
CS   Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455,
     USA
SO   Tetrahedron (2000), 56(36), 6603-6616
     CODEN: TETRAB; ISSN: 0040-4020
PB   Elsevier Science Ltd.
DT   Journal
LA   English
AB   We have been studying the artificial sweeteners aspartame
     (1-aspartyl-1-phenylalanine Me ester) and neotame
     (N-(3,3-dimethylbutyl)-1-asparty1-1-phenylalanine Me ester) as compds.
```

which exhibit polymorphism. 13C CP/MAS NMR shows that aspartame exists in three distinct forms at room temp., depending on prepn. conditions. For two of the forms, there exists three resonances for each carbon, indicating three crystallog. inequivalent sites and therefore three distinct conformations and/or arrangements of aspartame mols. within the unit cell. Two-dimensional exchange spectroscopy using high-speed MAS and very high-power 1H decoupling on uniformly 13C labeled aspartame is a very powerful tool for unambiguously assigning each resonance in the NMR spectrum of aspartame. Even for forms of aspartame that possesses multiple crystallog. inequivalent sites, it is possible to identify connectivities between the nuclei of each conformation and/or arrangement of mols. using two-dimensional NMR techniques. 13C CP/MAS NMR also shows that **neotame** exists in multiple solid forms. The most stable form of **neotame** under ambient conditions is a monohydrate. However, other forms can be prepd. by heating or using reduced pressures. High-speed magic-angle spinning can cause a change in polymorphic forms. Three different forms were produced upon spinning at 29 kHz for several days. The monohydrate was identified as the second form produced. Also, altering the crystn. and drying conditions can generate mixts. of the solid forms of **neotame**. When the monohydrate form of **neotame** was heated under vacuum, a mixt. of **anhydrate** forms was produced. In the reconversion to the monohydrate upon exposure to moisture under ambient conditions no significant changes were obsd. in the powder X-ray diffraction patterns during part of the reconversion process. This suggests that no change in form had occurred. The 13C CP/MAS NMR spectra, however, indicated the presence of many forms of **neotame** during the reconversion. One possible reason that solid-state NMR spectroscopy detected the changes in forms and powder X-ray diffraction did not is that the conformation of the **neotame** mols. changes between forms but the unit cell parameters do not change significantly.

RE.CNT 47

RE

(1) Andrew, E; Prog NMR Spectrosc 1971, V8, P1 CAPLUS
(2) Anon; US 5510508 CAPLUS
(3) Anon; US 5728862 CAPLUS
(4) Anwar, J; J Pharm Sci 1989, V78, P337 CAPLUS
(5) Bennett, A; J Chem Phys 1992, V96, P8624 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2001 ACS

TI Crystal structure and physical characterization of **neotame** methanol solvate

AN 2000:258873 CAPLUS
DN 133:59068

TI Crystal structure and physical characterization of **neotame** methanol solvate

AU Dong, Zedong; Young, Victor G., Jr.; Padden, Brian E.; Schroeder, Steve A.; Prakash, Indra; Munson, Eric J.; Grant, David J. W.
CS Department of Pharmaceutics, College of Pharmacy, University of Minnesota, Minneapolis, MN, 55455-0343, USA

SO J. Chem. Crystallogr. (1999), 29(8), 967-975
CODEN: JCCYEV; ISSN: 1074-1542
PB Kluwer Academic/Plenum Publishers
DT Journal
LA English

AB The crystal structure of the methanol solvate (empirical formula: 2C20H30N2O5.cntdot.3MeOH) of the dipeptide sweetener **neotame**,

N-(3,3-dimethylbutyl)-L-.alpha.-aspartyl-L-phenylalanine Me ester, was detd. [a = 9.8989(1), b = 18.1331(1), c = 27.5725(1) .ANG., orthorhombic, space group P212121, Z = 4]. Each unit cell includes 8 **neotame** and 12 MeOH mols. Disorder exists in one **neotame** mol. and one MeOH mol. The crystals were characterized by the following techniques: hot-stage microscopy (HSM), Karl-Fischer titrimetry (KFT), powder x-ray diffractometry (PXRD), differential scanning calorimetry (DSC), thermogravimetry (TGA), and 13C solid-state NMR (SSNMR). Under HSM at a heating rate of 10.degree./min, the sample melts at 64-84.degree. and liberates bubbles at 71-86.degree.. DSC in open pans shows two overlapping endotherms at 56 and 71.degree., probably due to melting and desolvation, resp. TGA in open pans shows 5.9% wt. loss due to desolvation below 70.degree.. Under 23 mmHg over P4O10 at 23.degree., the MeOH solvate produces pure amorphous **anhydrate**, which converts to cryst. **neotame**.H2O in the presence of moisture.

RE.CNT 21
RE
(1) Andrew, E; Prog NMR Spec 1971, V8, P1 CAPLUS
(3) Anon; US 5728862 CAPLUS
(5) Blessing, R; Acta Crystallogr 1995, VA51, P33 CAPLUS
(6) Dixon, W; J Magn Res 1982, V49, P341 CAPLUS
(7) Goodman, M; J Peptide Sci 1998, V4, P229 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	18.24	61.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.35	-5.88

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